Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.45e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.79e-01

Confidence level: 6.86e-01

Nearest Neighbors from the Training Set

Image not found
Guanidine, (2-benzothiazolyl)-
Measured: 3.62e-03
Predicted: 2.64e-03

Image not found
Isocil
Measured: 8.70e-03
Predicted: 5.23e-03

Image not found
Bromacil
Measured: 3.12e-03
Predicted: 3.11e-03

Image not found
Methabenzthiazuron
Measured: 2.67e-04
Predicted: 1.49e-03